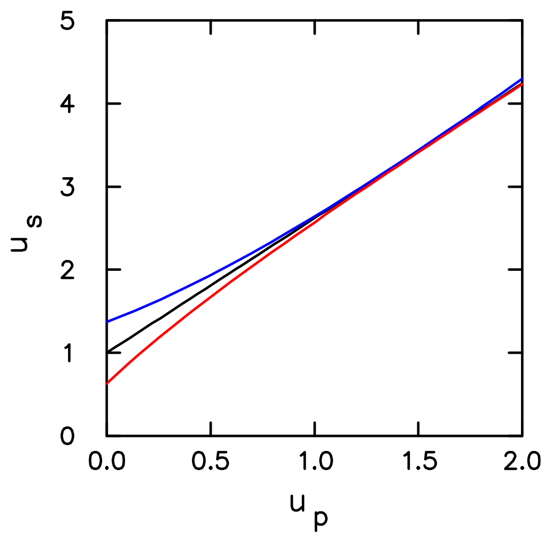
The shape of the Hugoniot locus in the (particle velocity, shock velocity)-plane at low pressures

RALPH MENIKOFF, T-14



- Convex
  Ideal gas
- Linear u_s–u_p approximation
  Approximation used for many metals
- Concave
  Foams & porous solids
  Liquids, molecular crystals & polymers

Outline

- Liquids (Glycerin, Water, Carbon Tetrachloride)

  A ”Universal” Hugoniot for Liquids

  R. W. Woolfolk, M. Cowperthwaite and R. Shaw

  Therochimica Acta 5 (1973) pp. 409-414

- Molecular Crystals (HMX)

  Fitting Forms for Isothermal Data

  Ralph Menikoff & Tommy Sewell

  `http://t14web.lanl.gov/Staff/rsm/preprints.html#IsothermFit`

- Polymer (estane)

  Equation of State and Hugoniot Locus for Porous Materials:

  P–α Model Revisited

  Ralph Menikoff & Ed Kober

  `http://t14web.lanl.gov/Staff/rsm/preprints.html#Porous`

- Thermodynamically consistent (equilibrium) EOS

  Based on P–α Model and two-phase flow

  • Constitutive Equation for the Dynamic Compaction of Ductile Porous Material

  W. Herrmann, J. Applied Phys. **40** (1969) pp. 2490–2499.

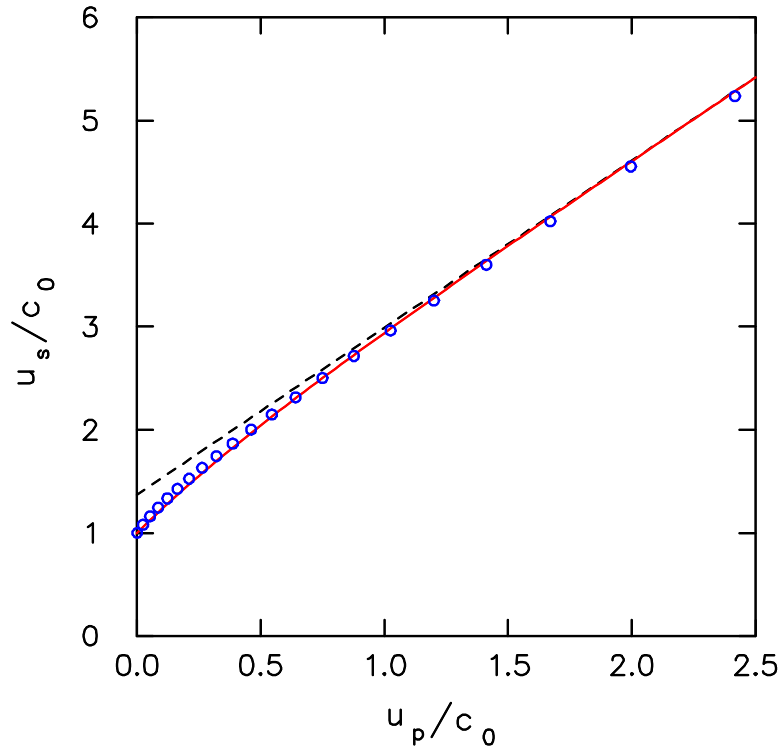
  • Suggested Modification of the P–α Model for Porous Materials

  M. Carroll & A. C. Holt, J. Applied Phys. **43** (1972) pp. 759–761.

  • A Two-Phase Mixture Theory for the Deflagration-to-Detonation Transition in Reactive Granular Materials

  M. R. Baer & J. W. Nunziato, Int. J. Multiphase Flow **12** (1986) pp. 861–889.

“Universal” Hugoniot for liquids



Red line, $\boxed{u_s \text{ function of } u_p}$

Empirical fit Woolfolk, Cowperthwaite & Shaw

$$u_s/c_0 = 1 + 1.62 * u_p/c_0 + \boxed{0.37\,[1 - \exp(-2u_p/c_0)]}$$

Blue symbols, $\boxed{u_s^{-1} \text{ function of } u_p/u_s}$

$$c_0/u_s = \frac{1 - 1.62 * (u_p/u_s) + 0.37\,\exp[-8(u_p/u_s)]}{1.37}$$

Asympototically, large u_p

$$u_s = 1.37 c_0 + 1.62 u_p$$

Mie-Grüneisen Equation of State

$$P(V,e) = P_h(V) + \frac{\Gamma}{V}\Big[e - e_h(V)\Big]$$

with **principal Hugoniot as reference curve**. Jump conditions

$$\begin{aligned} u_p/u_s &= 1 - V/V_0 \\ u_p &= (1 - V/V_0)\cdot u_s \\ P_h &= P_0 + \rho_0 (u_p/u_s) u_s^2 \\ e_h &= e_0 + 0.5\,(P_h + P_0)(V_0 - V) \end{aligned}$$

More efficient to evaluate $P_h(V)$

when u_s is function of u_p/u_s rather than u_p/c_0.

- u_s only requires function evaluation
- Do not solve equation for u_p given V.

Assumes P_h parameterized by V

- V is monotonic along principal Hugoniot locus.
- Required when Γ independent of e

$$\begin{aligned} e - e_0 &= \tfrac{1}{2}(V_0 - V)(P - P_0) \qquad \text{Hugoniot Equation} \\ &= \tfrac{1}{2}(V_0 - V)\cdot\left(P_h(V) - P_0 + \frac{\Gamma}{V}\Big[e - e_h(V)\Big]\right) \end{aligned}$$

$$\boxed{e - e_h(V) = \tfrac{1}{2}(V_0 - V)\cdot\frac{\Gamma}{V}\Big[e - e_h(V)\Big]}$$

Only one solution unless $\frac{\Gamma(V_0 - V)}{2V} = 1$, in which case, solution for all e.

Comment on generalizing linear u_s–u_p relation

Source unknown (guess LLNL or Univ. of Calif.)

Start with linear u_s–u_p relation

$$u_s = c_0 + s\,u_p$$
$$\frac{c_0}{u_s} = 1 - s\cdot\left(\frac{u_p}{u_s}\right)$$

Generalize to

$$\frac{c_0}{u_s} = 1 - \sum_n s_n\cdot\left(\frac{u_p}{u_s}\right)^n$$
$$\frac{c_0}{u_s} = 1 - \sum_n s_n\cdot\left(1-\frac{V}{V_0}\right)^n$$
$$\boxed{P_h(V) = \frac{\rho_0 c_0^2\left(1-\frac{V}{V_0}\right)}{\left[1-\sum_n s_n\cdot\left(1-\frac{V}{V_0}\right)^n\right]^2}}$$

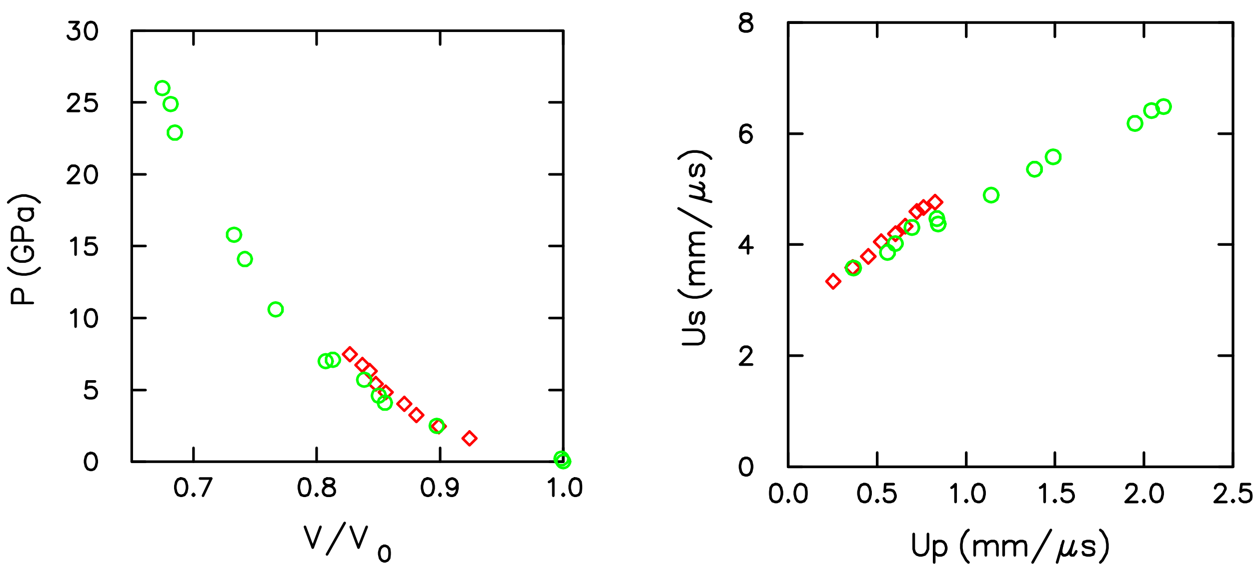
Better to use cubic spline for $u_s^{-1}(V)$

- Finite region in V
  Zero of $u_s^{-1}(V)$ corresponds to maximum shock compression
  Asymptotically linear u_s–u_p relation
- Avoids oscillations of polynomials
- Sound speed is continuous (no phase transition)
  Not true for piecwise linear fits that are sometimes used.

HMX isothermal data

1. Olinger, Roof. and Cady
   The linear and volume compression of β-HMX and RDX, in *Proc. Symposium (Intern.) on High Dynamic Pressures*, [C.E.A., Paris, France, 1978], pp. 3–8.

2. Yoo and Cynn
   Equation of state, phase transition, decomposition of β-HMX, *J. Chem. Phys.* **111**, pp. 10229–10235.



a) (V,P)-plane. b) (u_p,u_s)-plane.

diamonds are data from Olinger, Roof & Cady

circles are data from Yoo & Cynn

pseudo-velocities

- shock velocity
  $$u_s = V_0 \left[\frac{P-P_0}{V_0-V}\right]^{\frac{1}{2}}$$
- particle velocity
  $$u_p = [(P-P_0)\cdot(V_0-V)]^{\frac{1}{2}}$$

Fitting Forms

- Hugoniot form

  $$P(V) = \frac{V_0 - V}{\left[V_0 - s_T(V_0 - V)\right]^2} c_T^2$$

- Birch-Murnaghan

  $$P(V) = \frac{3}{2} K_{T_0} \left[\eta^{-7/3} - \eta^{-5/3}\right] \left[1 + \frac{3}{4}(K'_{T_0} - 4)(\eta^{-2/3} - 1)\right]$$

  where $\eta = V/V_0$

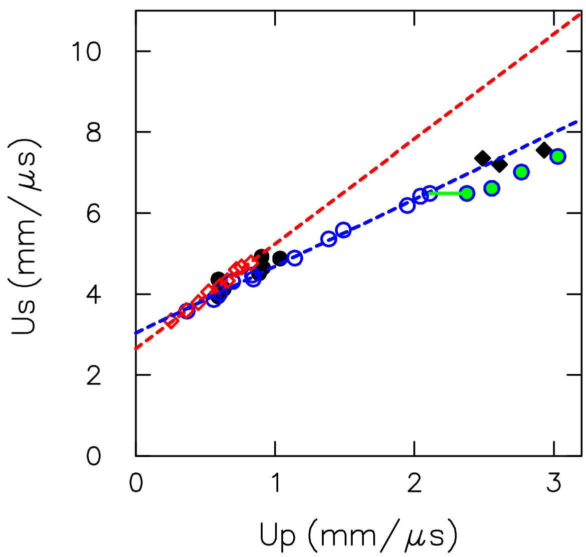
Both fitting forms have two parameters

(values at inital state)

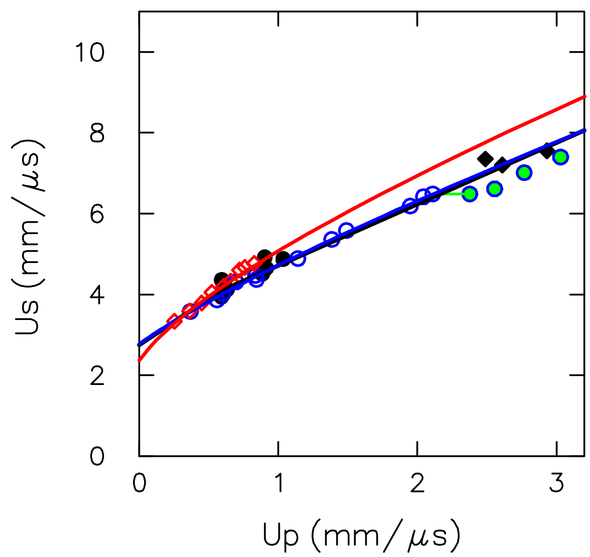
c & s for Hugoniot form

K & K' for Birch-Murnaghan form

Fits to Data



a) Hugoniot fits.



b) Birch-Murnaghan fits.

Red diamonds:	Olinger, Roof & Cady data.
Blue circles:	Yoo & Cynn data.
Black circles:	Hugoniot data, solvent pressed HMX (0.5% porosity)
Black diamonds:	Craig's single crystal Hugoniot data.

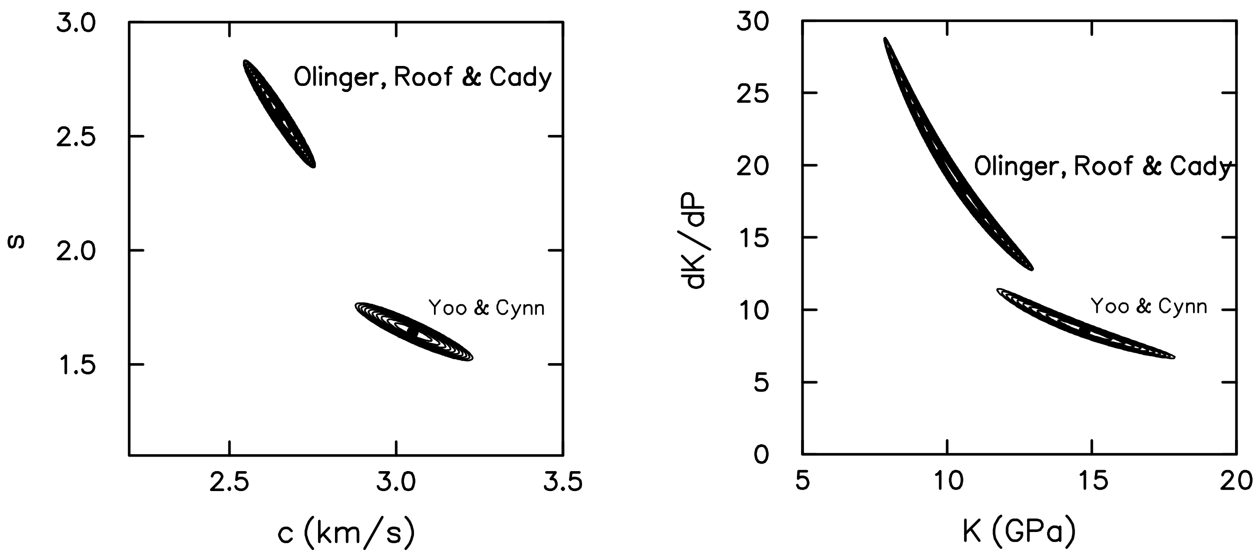
Dashed lines are **linear fits**
Solid lines are **Birch-Murnaghan fits**

Green above high pressure phase transition, 27 GPa

CJ detonation velocity $U_s \approx 9\,\mathrm{mm}/\mu s$

Shock temperature $\sim \frac{U_p^2}{2C_V}$

Reduced χ^2 of fits



a) Hugoniot fits. b) Birch-Murnaghan fits.

Sensitivity to statistical errors

- Can not distinguish fits based on χ^2
- Outter error “ellipse” is ~ 1 standard deviation
- Variation in parameters are corrolated
- Statistical significant difference in data sets
- Statistical significant diffence in fitting forms

Curvature of $U_s(u_p)$ locus

Curvature is common

Due to squeezing out “free volume”

1. Molecular crystals

   Example: PETN, HMX

2. Plastics or polymers

   Example: estane

3. liquids

   Example: water, alcohol

4. Porous materials and foams

Metals are “exceptions”

Atomic crystals

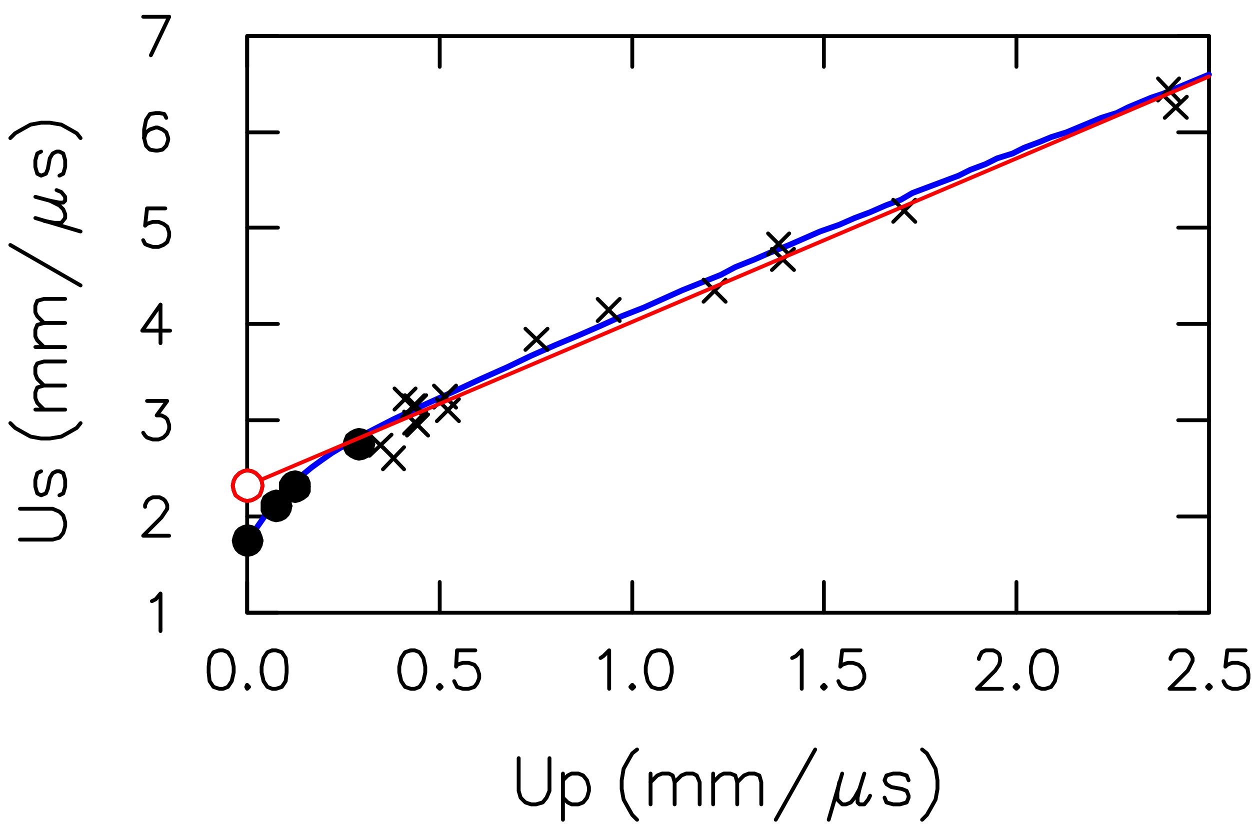
Material strength affects Hugoniot locus at low pressure

Explosives typically are large molecules

Expect stiffening P $\sim$ few kb

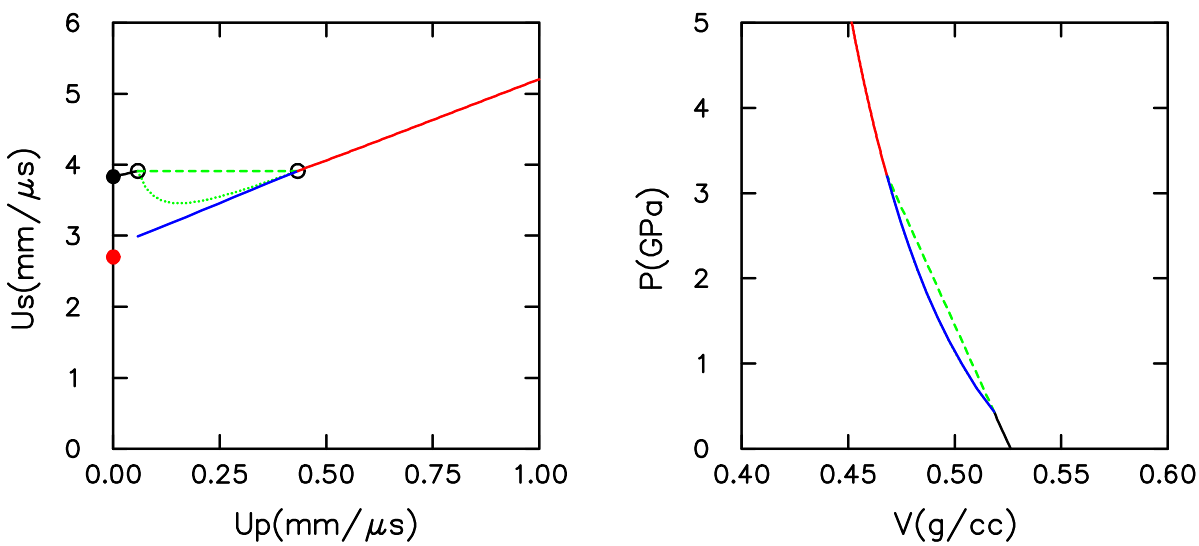
Compatible with bond bending energy $\sim$ 0.1 ev

Estane Hugoniot locus



Data points are denoted by the <u>symbol X</u>, [Marsh], and by a <u>solid circle</u>, [Dick]. The blue line is the Hugoniot locus computed from the porous equilibrium equation of state. The red line is a linear fit to Marsh's data. The open circle is sound speed corresponding to linear fit.

Elastic-Plastic Hugoniot loci



Comments

- Elastic-Plastic transition
  Single shock in green region is unstable
  Blue line corresponds to second shock in split wave

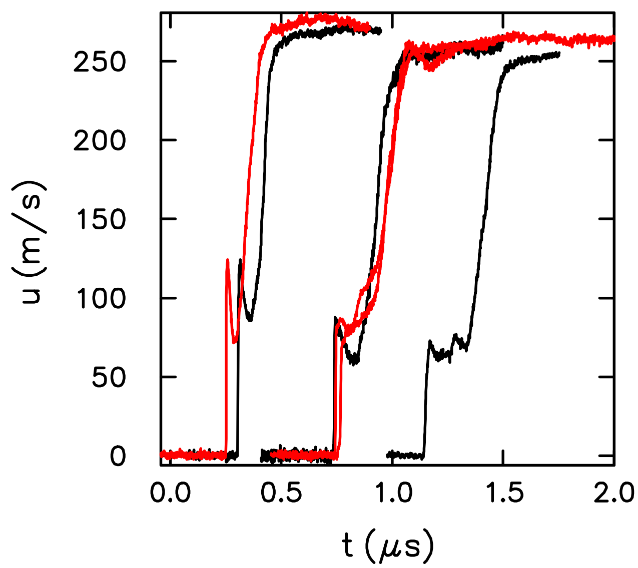
- Extrapolate high pressure (red region) loci til it intercept $u_p = 0$
  Typically, intercept slightly higher than bulk sound speed
  In contrast, for concave loci the discrepancy with intercept is larger

- Shock experiments
  Typically in strong single shock region
  in order to neglect strength effects

- Quasi-static compression vs. Shock compression
  Isotropic stress vs. Uniaxial strain

Sample wave profiles

HMX single crystal data, Jerry Dick DX-1



Comments

- Two-wave structure is evident
- Transient

  Elastic precursor decays
- Asymptotic state

  Requires relatively long run distance

Construct EOS for materials whose principal Hugoniot locus is concave

- Helmholtz free energy with internal variable ϕ

  Equilibrium ϕ minimizes free energy

  Degree of freedom used to fit Hugoniot locus.

- Thermodynamically consistent version of Herrmann-Carrol-Holt P–α model

  Complete EOS satisfing identity

  $\boxed{de = -PdV + T d\eta}$

- Analogy with reactive EOS

  Partial Hugoniots, fixed ϕ

  similar to endothermic reaction

- Example

  Estane, polymer used in binder of PBX-9501

  Can interpret $1-\phi$ as “free volume” $\lesssim 1.5\%$

Ansatz for free energy

$$\boxed{\Psi(V,T,\phi) = \Psi_s(\phi V,T) + B(\phi)}$$

Assume $B(\phi)$ strictly increasing and convex.

For porous material ϕ is volume fraction.

Thermodynamic relations

- Entropy

  $\eta = -\partial_T \Psi = \eta_s(V_s,T)$

  where $V_s = \phi V$

- Energy

  $e = \Psi + T\eta = e_s(V_s,T) + B(\phi)$

- Pressure

  $P = -\partial_V \Psi = \phi P_s(V_s,e_s)$

- Equilibrium ϕ

  Minimize free energy, $\partial_\phi \Psi = 0$

  $V_s P_s = \phi \frac{d}{d\phi} B(\phi)$

  defines $\phi = \phi_{eq}(V_s P_s)$

Equilibrium EOS

$$\Psi_{eq}(V,T) = \Psi(V,T,\phi_{eq})$$

Satisfies thermodynamic identity

$$de = -PdV + Td\eta$$

- Pressure

  $\boxed{P(V,e) = \phi P_s(\phi V, e - B(\phi))}$

- Equilibrium

  $\boxed{\phi = \phi_{eq}(V_s P_s)}$ or $P_s \approx \beta(\phi)$

  $\phi(V,e)$ defined implicitly as solution to

  $VP_s(\phi V, e - B(\phi)) = \frac{d}{d\phi}B(\phi)$

- Extra energy term

  $\boxed{B(\phi) = \int_{\phi_0}^{\phi} \phi_{eq}^{-1}(\phi)\frac{d\phi}{\phi}}$

Modification of Herrmann-Carrol-Holt P–α model.

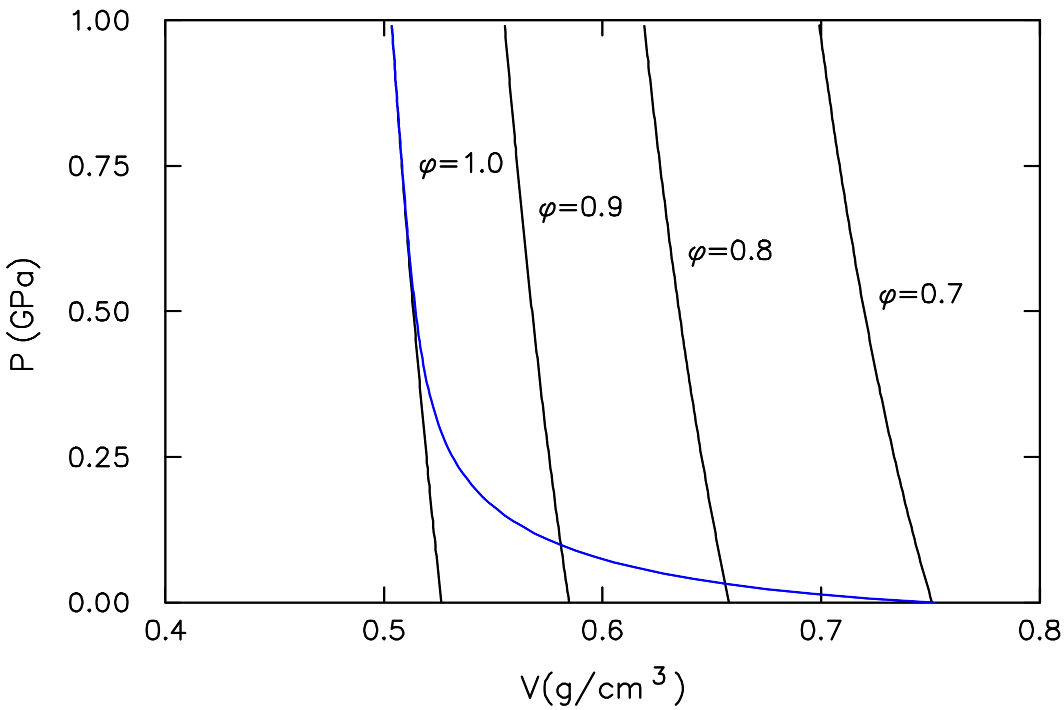
$\alpha = 1/\phi$ is "distension"

Sound speed, $c^2 = (\partial/\partial\rho)P|_\eta$

$$\left(\frac{c}{c_s}\right)^2 = 1 - \left(\frac{\gamma_s - 1}{\gamma_s}\right)^2 \frac{c_s^2}{c_s^2 + \phi^2(d^2/d\phi^2)B}$$

where $\gamma_s = \rho_s c_s^2/P_s$ and $c_s^2 = (\partial/\partial\rho_s)P_s|_\eta$

Partial Hugoniot loci



black lines are loci with fixed ϕ

blue line is locus with ϕ_{eq}

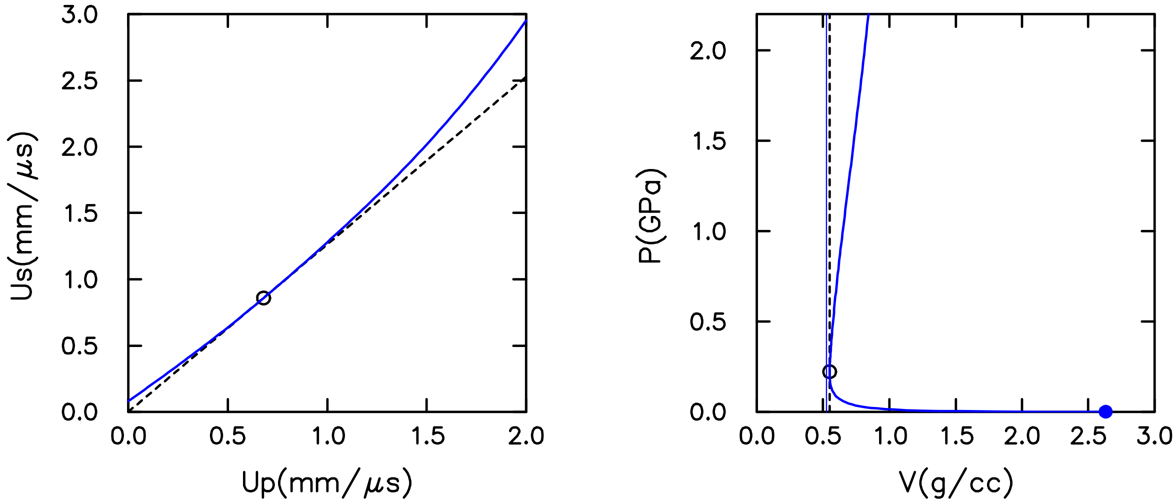
With increasing ϕ loci in (V, P)-plane shifts to left. Analog of endothermic reaction.

However, pressure dominated by dependence on V rather than energetics.

For fixed P, increasing ϕ lowers u_s and raises u_p

Choose ϕ_{eq} to give desired $u_s(u_p)$.

Example of Hugoniot loci for highly porous material



Comments

- 80 % porosity (aero-gel)

- V non-monotonic

  V_0 (of pure solid) $< V$, thermal pressure is dominant

  Hence porous Γ not independent of e, pure solid is

- u_p–u_s locus is convex

  Tangent line at $dP/dV = 0$ goes through origin

Ref: Zel'dovich & Raizer

Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena, Vol II

Chpt. XI, sec. 10, Shock compression of porous materials

Equilibrium vs. Non-equilibrium

- Equilibrium EOS

  Quasi-static compression is reversible, e.g. liquid

  Path independent with only entropy

- Non-Equilibrium

  Irreversible, crush-up of porous solid

  Need to introduce internal variables & rate equations

  - Chemical reactions

    λ, Reaction progress variables & Reaction rate

  - Plasticity

    Plastic strain & Plastic strain rate

  - Porosity or 'free volume'

    Split volume fraction, $\phi = \phi_{elastic} + \phi_{plastic}$

    Compaction equation, $\partial_t + \vec{u} \cdot \nabla\phi = (P_s - \beta)/\mu$,

    and similarly for $\phi_{plastic}$

    Dissipation, $T\frac{ds}{dt} = \frac{V\,(P_s-\beta)^2}{\mu}$

Partly dispersed waves at low pressures

    Ref: Gonthier, Menikoff, Son & Asay

    Modeling compaction-induced energy dissipation of granular HMX

    Proceedings of the 11th Detonation Symposium, 1998, pp. 153-161